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First-principles calculation of exchange interaction and exchange force between magnetic Fe films

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Abstract

First-principles calculations have been performed for the exchange interaction and exchange force between two magnetic Fe(100) thin films. It is shown that the magnitude of the calculated exchange force is of the order of 10^{-9}N at $d/a < 1$ and of the order of 10^{-10}N at $1 < d/a < 1.5$, where d denotes the distance between surfaces of the two thin films and a the lattice constant of bulk Fe. The obtained forces are sufficiently larger than the sensitivity of the current atomic force microscopy of $10^{-12} - 10^{-13}$N, which suggests the feasibility of the *exchange force microscopy*.

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I. INTRODUCTION

Surface magnetism has attracted much attention both in fundamental and applied researches. Experimental techniques to investigate the magnetic structure of the surface having been developed, mainly detect the spin polarization of electrons emitted from surface and the average magnetization on sample surface within a sub-micron range is usually observed. None of the techniques has so far probed the local magnetic structure in an atomic scale.

The scanning tunneling microscopy (STM)[1] and the atomic force microscopy (AFM)[2] provide us with a way to investigate the surface structure with atomic resolution. The STM probes the surface of conducting materials by measuring tunneling current between the tip and sample, whereas the AFM senses the atomic force between them. The AFM has a great advantage that it can be applied not only to conducting materials but also to insulators. The extension of the STM to measurements of the magnetic structure, the so-called spin-polarized STM (SP-STM), is currently being developed by various groups with different approaches.[3–5]

The magnetic force microscopy (MFM)[6] detects the force arising from the long-range interaction between magnetic dipoles of the tip and sample. The typical tip-sample separations in the MFM are of the order of more than 10nm and the spatial resolution is of the order of 10nm to 100nm. It is fairly certain that improvement of the resolution might be made by probing the short-range exchange force rather than the long-range magnetic dipole force.[7–9]

In previous papers,[7,8] we pointed out the possibility of the *exchange force microscopy* (EFM) which probes the short-range exchange force between the tip and sample. Since microscopic understanding of the exchange interaction between the tip and sample is of great importance and crucial in designing the EFM, we previously studied the exchange interaction between ferromagnetic tip and ferromagnetic sample based on a one-dimensional electron gas model.[7,8] By using a tight-binding model, Ness and Gautier[9] calculated the exchange interaction between a ferromagnetic Fe tip and magnetic Cr(001) and Ni(001)

surfaces. Since these calculations inevitably employ semi-phenomenological parameters, it is highly desirable to make *quantitative* evaluation of the exchange interaction and the exchange force for more realistic systems on the basis of first-principles electronic structure calculations, which is the purpose of the present paper.

The paper is organized as follows: In Sec.II we discuss the adopted model and calculation method. The calculated results are presented in Sec.III. The final Sec.IV is devoted to conclusion and discussion.

II. METHOD OF CALCULATION

By modeling the tip and samples to be used in actual experiments, we adopt the two three-atomic-layer Fe(100) films which are separated by the distance d, as shown in Fig. 1. Surface atoms of the one film are assumed to be facing the hollow sites on the surface of the other film. The translational symmetry is preserved in the surface-normal (x) direction, in which a set of the two three-layer films are periodically located with the five-atomic-layer vacuum gap (repeated slab model). For a calculation of the electronic structure of the adopted films, we employ the local-spin-density approximation to the density-functional theory, and the linear augmented-plane-wave (LAPW) method[10] with Hedin-Lundquist exchange correlation.[11] The potential and charge density are expanded with plane waves in the whole space and with spherical waves inside muffin-tin spheres, and the force is calculated by following the prescription given by Soler and Williams.[12] Because bulk Fe is in the ferromagnetic ground state, magnetic moments in each three-layer film is taken to be in the ferromagnetic alignment. As far as the relative orientation of moments in the two films are concerned, however, we consider the parallel (P) and anti-parallel (AP) configurations in order to calculate the exchange interaction and the exchange force between the two magnetic films. Our LAPW calculations are carried out by changing the film-film separation d from 1.4Åto 5.0Åwith an assumption that the internal atomic coordinates of each film are rigidly fixed.

III. CALCULATED RESULTS

A. Magnetic Moments

We discuss first the magnetic moments in the adopted Fe thin films. Figure 2 shows the spin magnetic moments calculated within the muffin-tin spheres of Fe atoms in the three layers of the upper film, which are referred to as the x_1, x_2 and x_3 layers (Fig. 1). The film-film separation d in the abscissa is denoted relative to the lattice constant of bulk Fe (a = 2.83Å). We should note that the separation of $d/a = 0.5$ corresponds just to the interlayer distance of bulk Fe. Due to the symmetry in our model, the magnetic moments in the x'_n layer of the lower film are the same as those in the x_n layer of the upper film in the P configuration, while in the AP configuration those in the x'_n layer has the same magnitude but with the opposite sign as those in the x_n layer. For both P and AP configurations, the magnetic moments at the outer x_3 layer is enhanced to be about $2.9\mu_B$, which is almost identical to the surface magnetic moment obtained by slab calculations.[13,14] The magnetic moments at the central x_2 layer is about $2.3\mu_B$, which is close to the experimental bulk value and to calculated one at the central layer of the slab.[14] The magnetic moments of the x_2 and x_3 layers for both P and AP configurations are almost independent of the film-film separation. On the contrary, magnetic moments on the x_1 layer change considerably at $d < a$, where the magnetic moments reduce significantly from the surface value to the bulk one as decreasing d. Nevertheless, the change in the magnitude of moments of the x_1 layer becomes insignificant for $d/a > 1$. We notice that the magnetic moments for the AP configuration are always smaller than that for the P configuration.

B. Exchange Interaction

The total energies, $E_{\rm P}$ and $E_{\rm AP}$, for the P and AP configurations are shown in Fig. 3 as a function of d/a. When the films are moved from the bulk position at $d/a = 0.5$, the total energies for both $E_{\rm P}$ and $E_{\rm AP}$ increase. The exchange interaction energy, $E_{\rm ex}$, defined by $E_{\rm ex} = E_{\rm AP} - E_{\rm P}$ is also plotted in Fig. 3. In the all region ($0.5 < d/a < 1.7$) investigated, we get the positive $E_{\rm ex}$, which means that the P configuration is more favorable than the AP one. This is expected from the fact that the resulting magnetic configuration corresponds

to a natural stacking of ferromagnetic Fe in bulk. The exchange interaction energy has an RKKY-type oscillation[15] with a period of about $d/a = 0.7$ ($\sim$ 2Å). The peak values of E_{ex} are 0.35eV at $d/a = 0.6$ and 0.19eV at $d/a = 1.35$. Note that the exchange interaction can be realized even at relatively far separation at $1.4 < d/a < 1.8$ (4.0Å$< d <$5.0Å).

C. Exchange Force

Figure 4 shows the atomic forces acting on atoms at the x_1, x_2 and x_3 layers of the upper film. The force direction is perpendicular to the film surface due to symmetry. As in the case of magnetic moments (Fig. 2), the atomic force for the x_1 layer has a significant d dependence whereas forces for the x_2 and x_3 layers are almost independent of d. The total forces summed up these forces: $F = \sum_n F(x_n)$, for the P and AF configurations, are shown in Fig. 5. The exchange force defined by $F_{\rm ex} = F_{\rm AP} - F_{\rm P}$ has an oscillation against d/a with the period of about 0.7, which is identical with the period of the exchange interaction (Fig. 3). The magnitudes of the first and second peaks are 1×10^{-9} N and 2×10^{-10} N, respectively. In the case of $d/a < 1$, where the relevant d orbitals must have a large overlap, the exchange force may arise from the direct exchange couplings between d states of the two films. In the case of $d/a > 1$, on the other hand, the exchange coupling is expected to be mediated through delocalized s and p electrons.

IV. CONCLUSION AND DISCUSSION

In summary, we have performed the first-principles calculation of the exchange interaction and the exchange force between two magnetic Fe(100) thin films, to show that the magnitude of the calculated exchange force is of the order of 10^{-9} at $d/a < 1$ while it is of the order of 10^{-10}N at $1 < d/a < 1.5$. It has been shown that at $d > a$, the perturbation of the approaching ferromagnetic film to magnetic moments in the other film, is negligibly small. The calculated magnitude of the exchange force is in fairly good agreement with our previous result of $10^{-10} \sim 10^{-11} N$ in spite of a crudeness of the one-dimensional electron-gas model.[78] Our result is also comparable with the exchange force of $0.4 \times 10^{-9} N$ between a Fe

tip and Cr(100) surface calculated by Ness and Gautier[9] with the use of the tight-binding model. Because the sensitivity of the current AFM is of the order of 10^{-12} to 10^{-13}N[16] our calculation suggests the possibility of the EFM, although it would be necessary to take into account an actual shape of the apex tip before we deduce definite conclusions. Ness and Gautier have been pointed out[9] that magnitudes of the exchange energy and force do not strongly depend on the tip morphology, although tip's shape varies the tip-sample distance where exchange interaction and force have the maximum values. It has been also shown[9] from calculations adopting sharp and blunt tips that an atomically sharp tip is not necessary for an actual observation with a constant-force mode, although a sharp tip is indispensable for a high, lateral spatial resolution. These results[9] justify, to some extent, our calculation employing a thin film as a tip; a first-principles calculation adopting more realistic tips is under consideration.

In actual measurements of the surface magnetic structure by using the EFM, we would have the two possibilities: a constant-force mode and a constant-distance mode, just as in the STM.[1] In the constant-force mode, we detect the variation of the tip-sample distance due to the force difference between the parallel and anti-parallel configurations. Such a experiment[3] has been made to detect the antiferromagnetic structure from one terrace to the next on Cr(100) surface, by using the constant-current mode in the SP-STM. On the contrary, in the constant-distance mode, we directly detect a change of the exchange forces between the parallel and anti-parallel configurations at a given tip-sample separation. If such a measurement is performed by changing the tip-sample distance, we would face technical difficulties such as the snap-in effect: when the tip-sample distance comes in the point of force instability where the gradient of the force exceeds the magnitude of the lever stiffness, the tip and surface would snap into contact.[17] In order to measure the RKKY-type exchange force, we require an exploration of the way to avoid the snap-in effect. Recently, a continuous measurement of the force curve between tip and sample, as approaching towards contact without the snap-in effects, can be provided by means of force-controlled feedback system.[18] This technique may possibly provide the basis of the EFM measurement.

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FIGURES

FIG. 1. Schematic representation of the two three-atom-layer Fe (100) films adopted in our calculation, surface atoms of the one film facing the hollow sites on the surface of the other film. Open circles represent Fe atoms and the lines denote the layer planes which are referred to as the x_n and x'_n layers ($n = 1 - 3$).

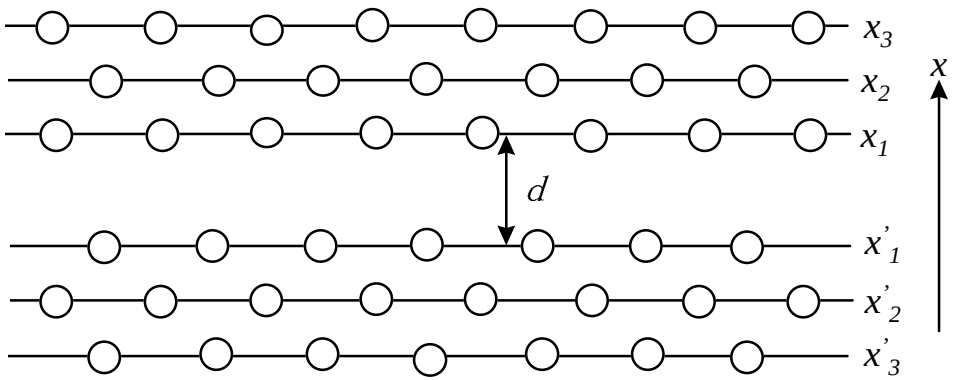
FIG. 2. Magnetic moments in the muffin-tin sphere of an Fe atom in the x_1 (circles), x_2 (triangles) and x_3 (squares) layers as a function of the film-film separation d normalized by the lattice constant of bulk Fe ($a = 2.83$Å). Solid and open marks stand for the P and the AP configurations, respectively.

FIG. 3. The film-film separation dependence of total energies in the P ($E_{\rm P}$: filled circles) and AF ($E_{\rm AF}$: open circles) configurations, and of the exchange energy defined by $E_{\rm ex} = E_{\rm AF} - E_{\rm P}$ (triangles). The reference energy for $E_{\rm P}$ and $E_{\rm AF}$ is the total energy for the P configuration at $d/a = 0.5$.

FIG. 4. Atomic forces, $F(x_n)$, acting on the atom of the x_n layer as a function of the film-film separation. Solid and open marks stand for the P and the AP configurations, respectively.

FIG. 5. The film-film separation dependence of total forces in the P ($F_{\rm P}$: filled circles) and AF ($F_{\rm AF}$: open circles) configurations, and of the exchange force defined by $F_{\rm ex} = F_{\rm AF} - F_{\rm P}$ (triangles).

Fig. 1, Nakamura, PRB



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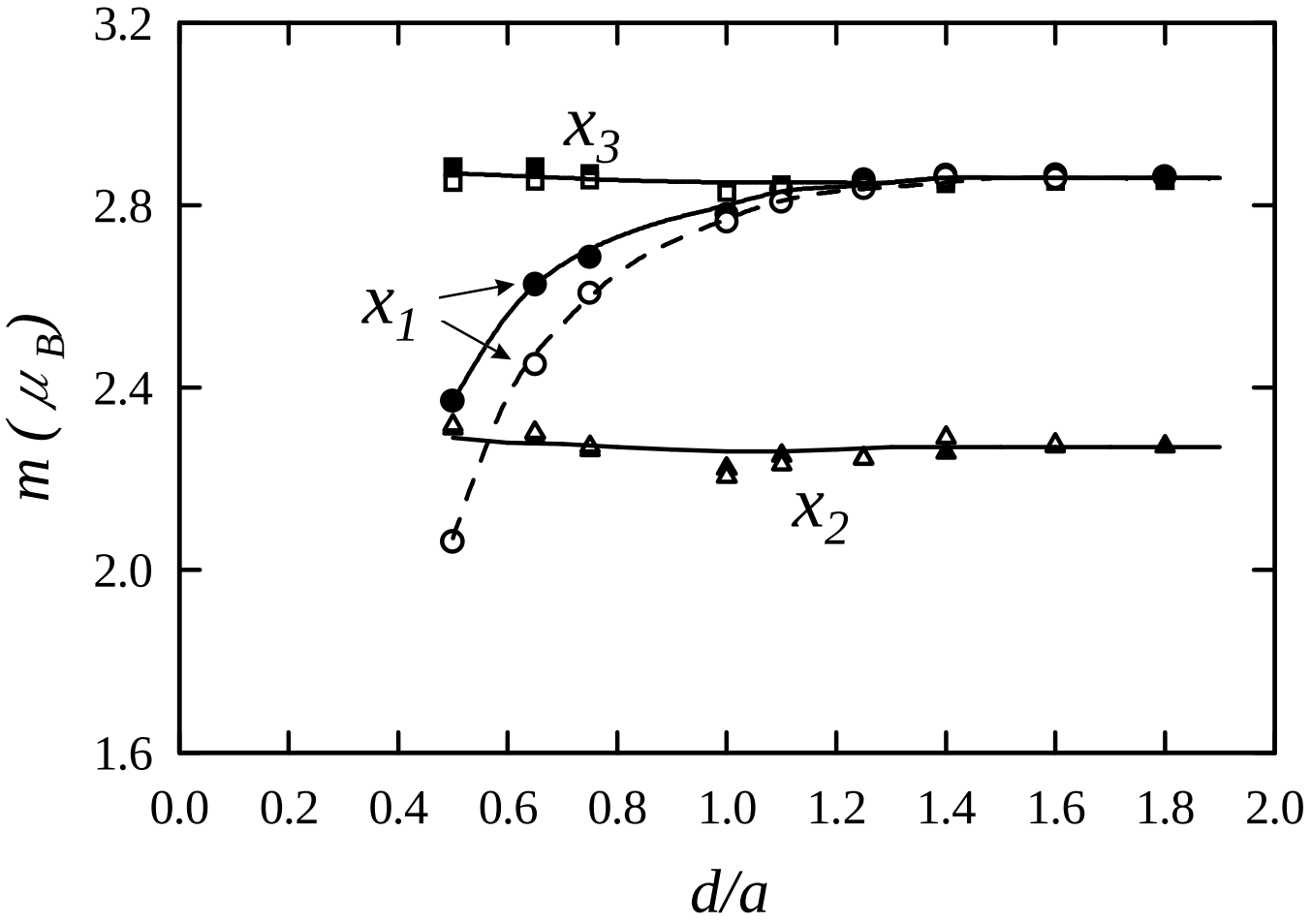

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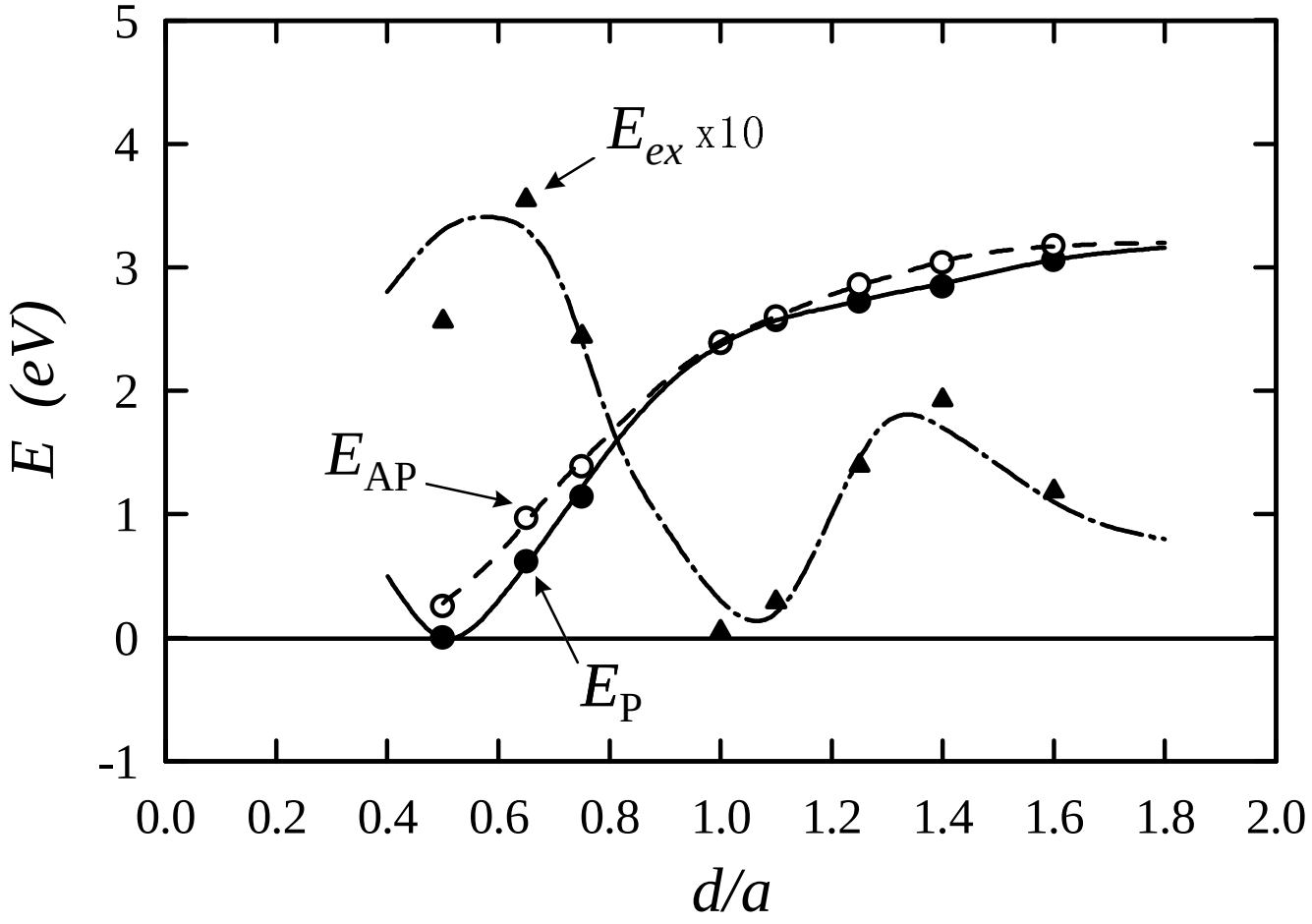

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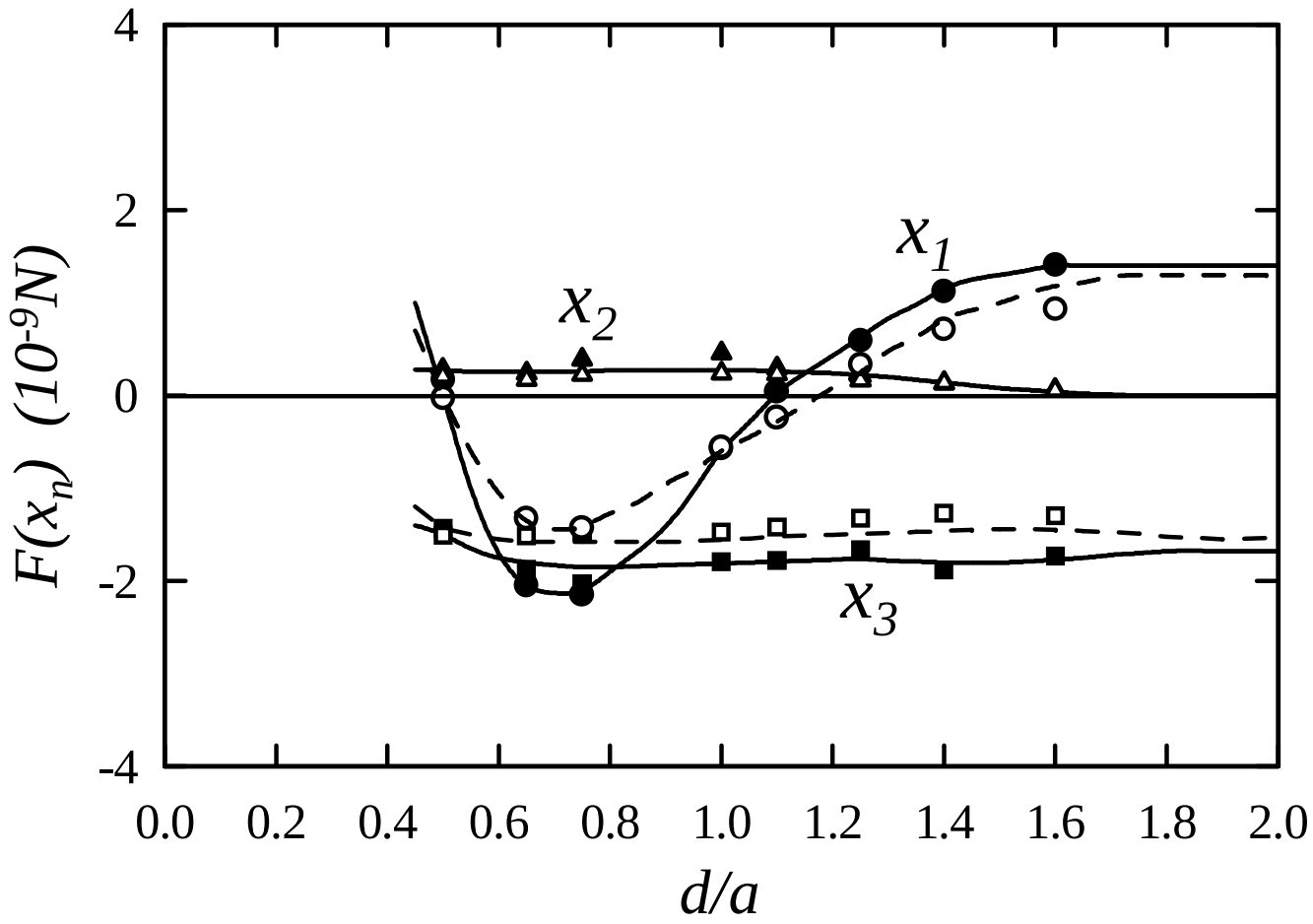
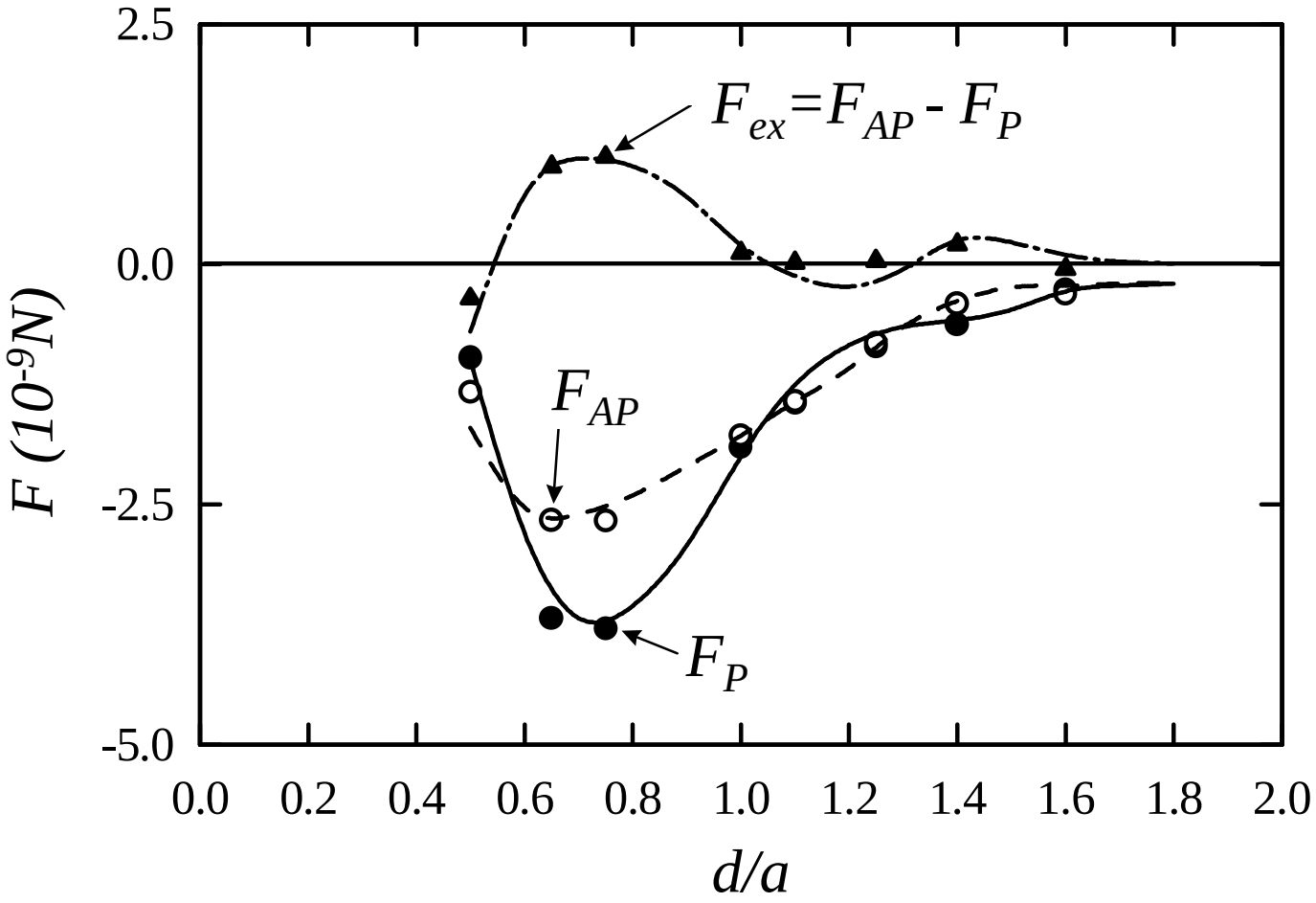
Fig. 5, Nakamura, PRB